

LA-UR-18-30196

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Title: Workflow for Alloy Design

Author(s): Rudin, Sven Peter

Intended for: Update during discussion at AFRL/Tech Engagement Office on "Improved Workflow for Alloy Design"

Issued: 2018-10-25

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Workflow for Alloy Design

Effect of dopants on
Ti phase stabilities

soft phonon modes connect
bcc and alpha/omega:
→ focus on lattice vibrations

Effect of dopants on
individual phonon modes

Effect of dopants on
phonon mode interactions

Effect of dopants on
high- T mode interactions

for C_D selected doping configurations...

... evaluate
 $3N$ phonon modes

... evaluate effect on
 $(3N)^2$ pairs of
frozen phonon modes

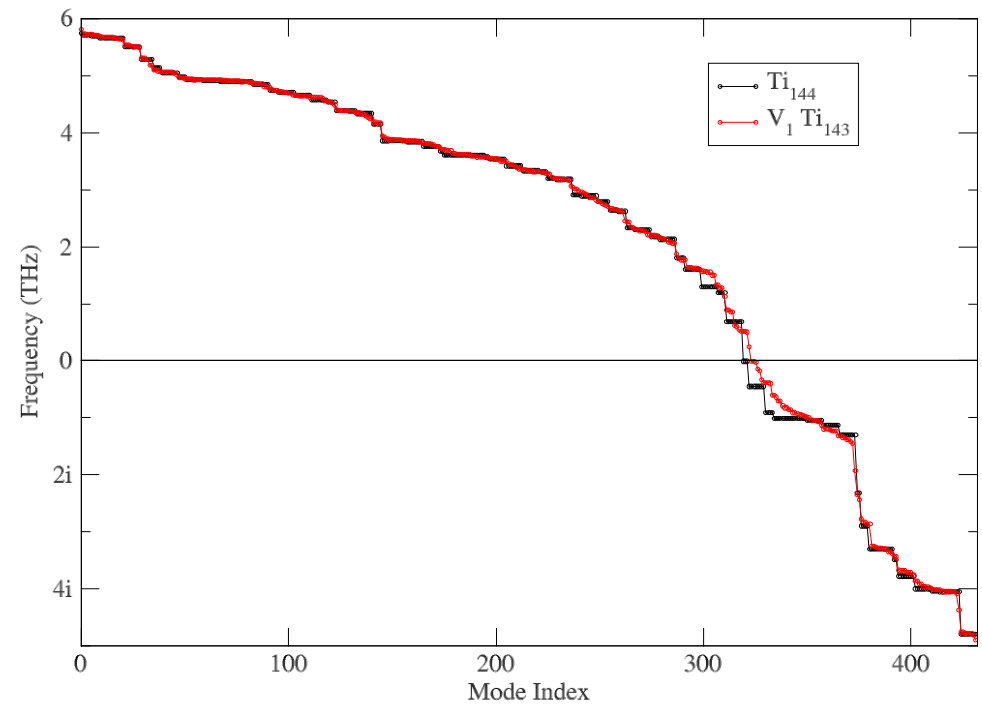
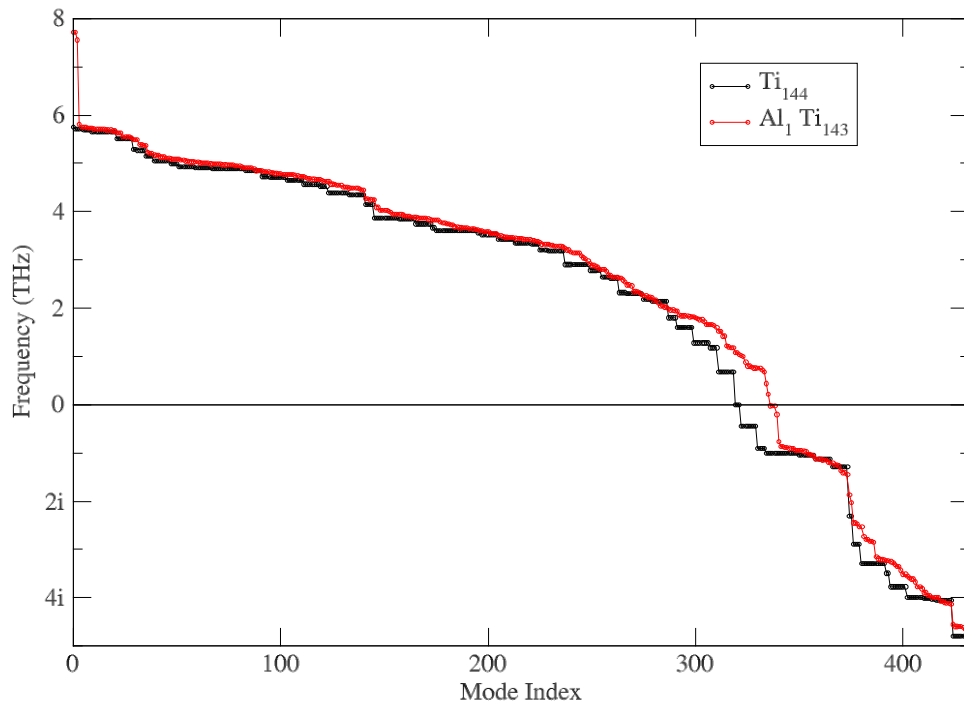
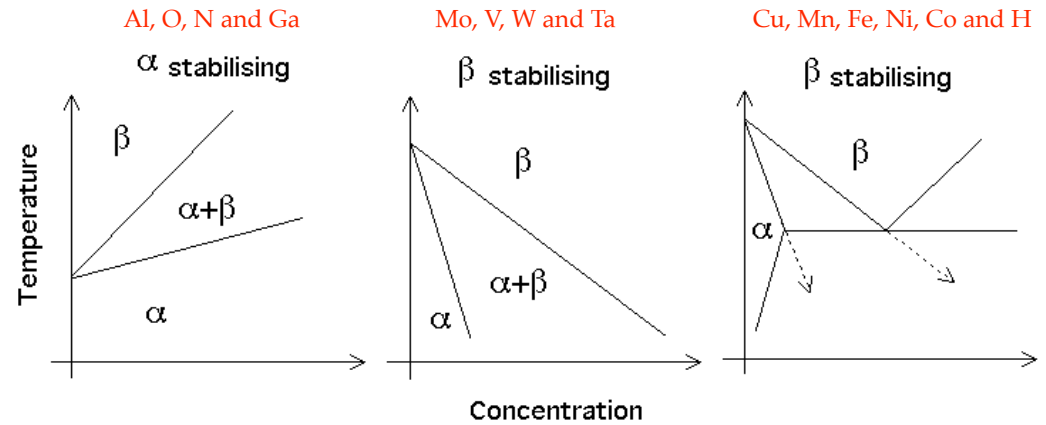
... run QMD,
perform PVM analysis

based on results, add additional doping configurations

Workflow for Alloy Design

for C_D selected doping configurations...

... evaluate
3N phonon modes

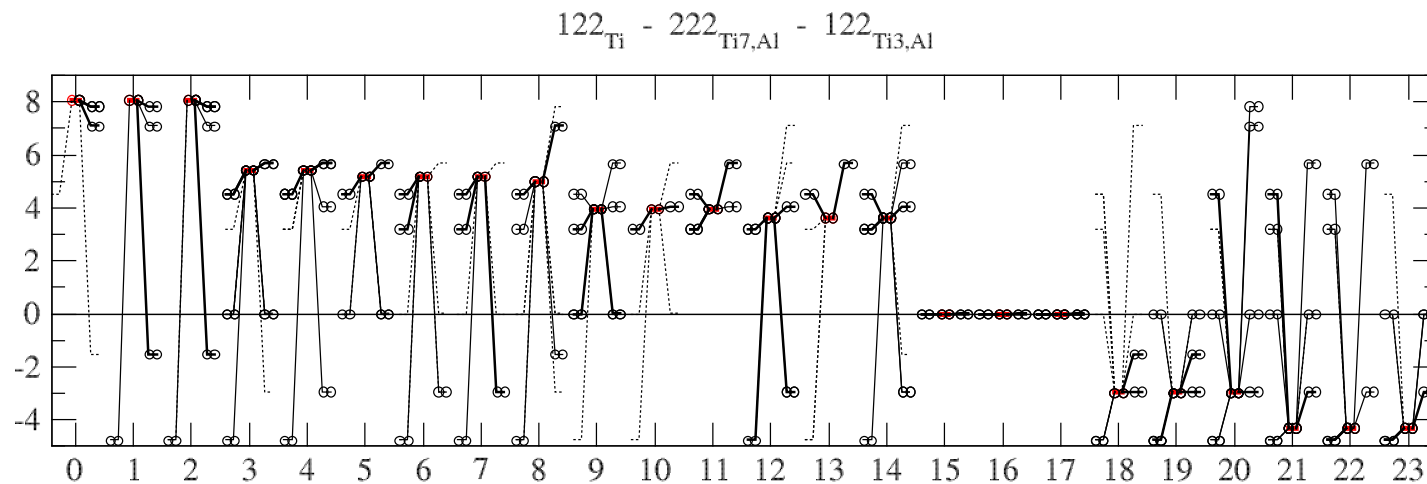
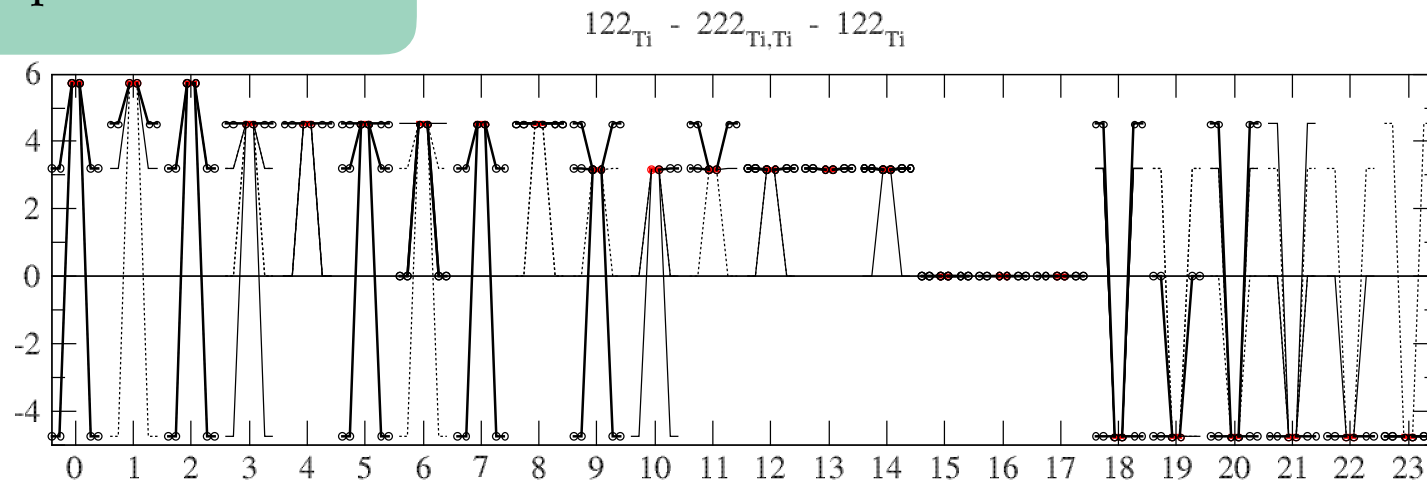


Workflow for Alloy Design

for C_D selected doping configurations...

... evaluate
3N phonon modes

Hierarchy of mapping supercell phonon modes onto
modes in smaller cell: hierarchical understanding?

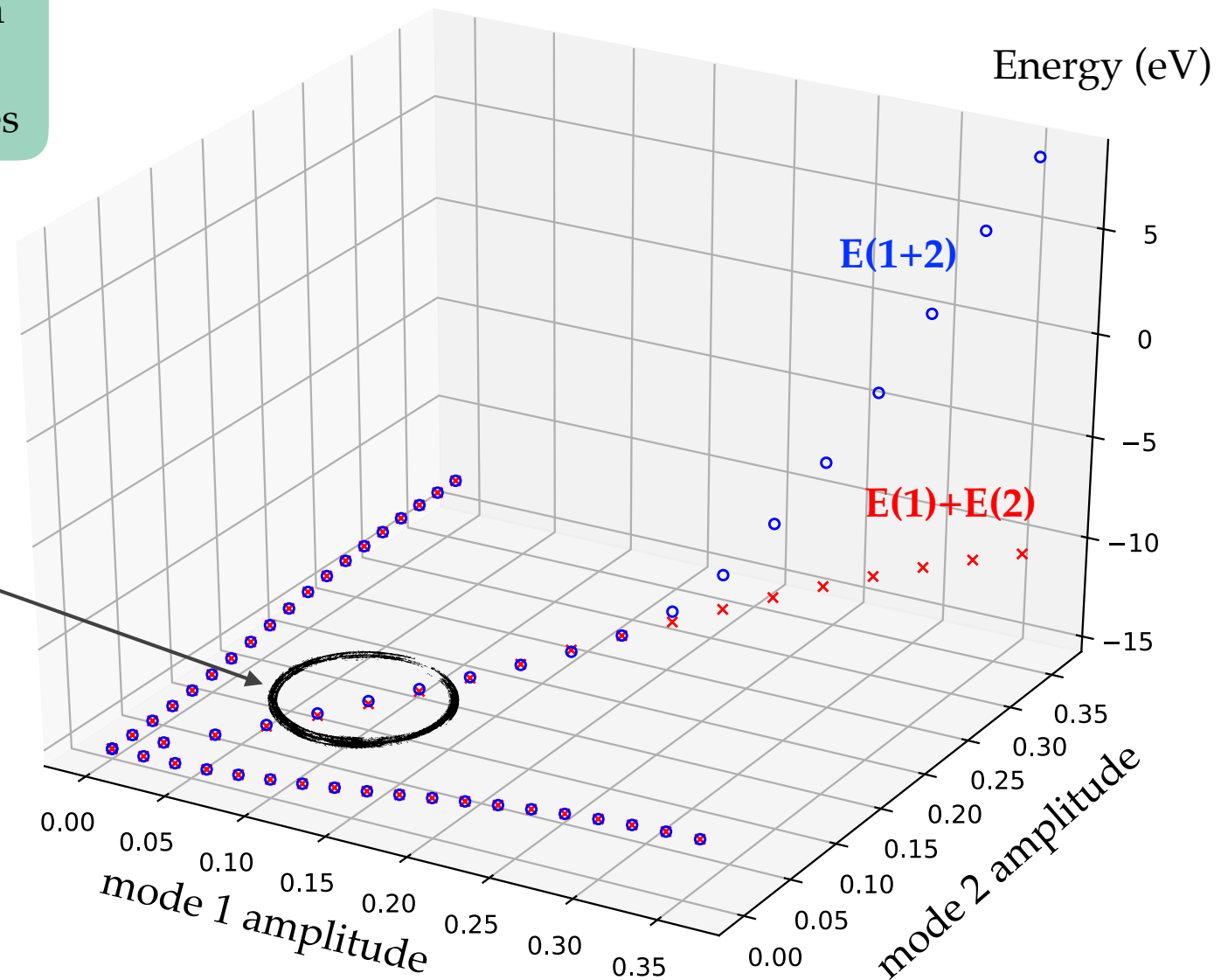


Workflow for Alloy Design

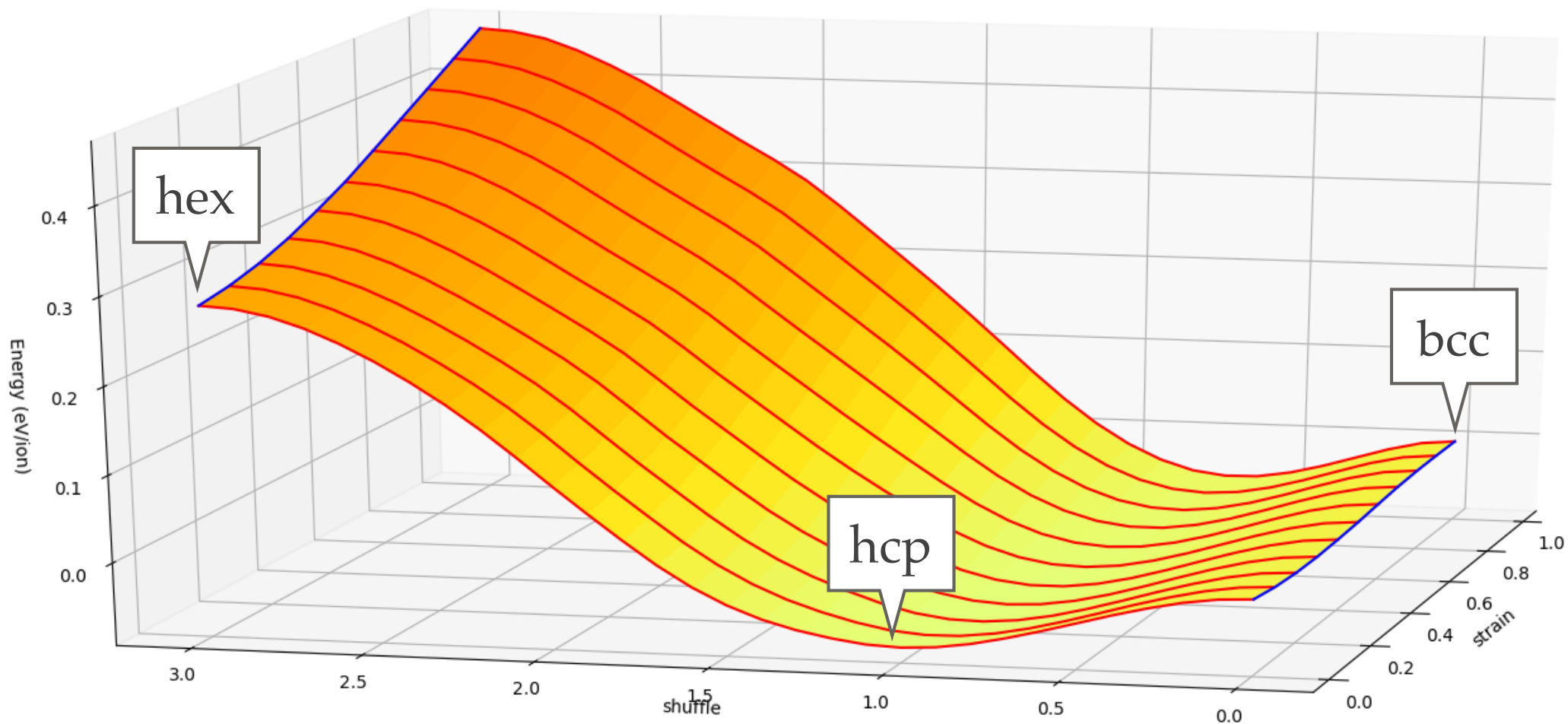
for C_D selected doping configurations...

... evaluate effect on
 $(3N)^2$ pairs of
frozen phonon modes

phonon—phonon
interaction



Workflow for Alloy Design



strain	shuffle	a/b		E(4)	-> E(144)	E(144) < Eigen	delta
0	0	0.57735026919		-30.5821	-1100.9538		
0	1	0.57735026919	"hcp"	-30.8629	-1111.0636	-1110.7111	-0.0024
1	0	0.707106781187	bcc	-30.5540	-1099.9430	-1099.7338	-0.0015
1	1	0.707106781187		-30.6196	-1102.3074	-1100.5692	-0.0121

Workflow for Alloy Design

for C_D selected doping configurations...

... run QMD,
perform PVM analysis

substitute one Ti in S144/Fcc
with Al

